Butyl 2-hydroxy-2-methylpropanoate 816-50-2 | DTXSID50278111

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.65 days

Global applicability domain: Inside

Local applicability domain index: 3.66e-01

Confidence level: 7.57e-01

Nearest Neighbors from the Training Set

Image not found

Tetradeca-1,13-diene
Measured: 367

Predicted: 8.69

Image not found

2,4-Dimethylheptane

Measured: 61.9 Predicted: 4.29

Image not found

2-Methylheptane

Measured: 12.5 Predicted: 3.99

Image not found

2-Methylhexane Measured: 12.5 Predicted: 5.54